Few-Body Systems manuscript No.
(will be inserted by the editor)

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Six-bodies calculations using the Hyperspherical Harmonics method

Received: date / Accepted: date

Abstract In this work we show results for light nuclear systems and small clusters of helium atoms using the hyperspherical harmonics basis. We use the basis without previous symmetrization or antisymmetrization of the state. After the diagonalization of the Hamiltonian matrix, the eigenvectors have well defined symmetry under particle permutation and the identification of the physical states is possible. We show results for systems composed up to six particles. As an example of a fermionic system, we consider a nucleon system interacting through the Volkov potential, used many times in the literature. For the case of bosons, we consider helium atoms interacting through a potential model which does not present a strong repulsion at short distances. We have used an attractive gaussian potential to reproduce the values of the dimer binding energy, the atom-atom scattering length, and the effective range obtained with one of the most widely used He-He interaction, the LM2M2 potential. In addition, we include a repulsive hypercentral three-body force to reproduce the trimer binding energy.

1 Introduction

The Harmonic Hyperspherical (HH) method is extensively used in the description of few-body systems. For example the HH method has been applied to describe bound states of $A = 3, 4$ nuclei (for a recent review see Refs. [1,2]). In these applications the HH basis elements, extended to spin and isospin degrees of freedom, have been combined in order to construct antisymmetric basis functions; in fact, the HH functions, as normally defined, do not have well defined properties under particle permutation, but several schemes have been proposed to construct HH functions with an arbitrary permutational symmetry, see Refs. [3,4,5,6].

All of the proposed symmetrization schemes share an increasing computational difficulty as the number of particles A increases; to cope with this issue, the authors proposed in Ref. [7] to renounce to the symmetrization step. If the Hamiltonian commutes with the group of permutations of A objects, S_A, the eigenvectors can be organized in accordance with the irreducible representations of S_A; in fact, if there is no more degenerancy, the eigenvectors have a well defined permutation symmetry. After the identification of the eigenvectors belonging to the desired symmetry, the corresponding energies are variational estimates. The disadvantage of this method results in the large dimension of the matrices

Presented at the Sixth Workshop on the Critical Stability of Quantum Few-Body Systems, Erice, Sicily, October 2011

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to be diagonalized. However, at present, different techniques are available to treat (at least partially) this problem.

In order to show the main characteristics of this method, we will discuss results for bound states up to six particles interacting through a central potential in two different systems: (i) a nucleon system interacting *via* the Volkov potential, used many times in the literature [5,8,9,10,11,12], and thus useful to test our approach, and (ii) a systems composed by helium atoms interacting through a soft-core potential. The *ab-initio*-helium potentials have a strong repulsion at small distances which makes calculations quite difficult; few calculations exist on clusters of helium with these potentials [13,14,15]. On the other hand, descriptions of few-atoms systems using soft-core potentials are currently operated (see for example Ref. [16,17,18]).

The paper is organized as follows. In Sect. 2 a brief description of the method is given. In Sect.3, applications of the method to a system of nucleons and helium atoms are shown. The conclusions are given in the Sect. 4.

2 The unsymmetrized HH expansion

In the present section we give a brief description of the HH basis showing some properties of the basis that allow to use unsymmetrized basis elements to describe a system of identical particles.

2.1 The HH basis set

Following Refs.[11,18,7], we start with the definition of the Jacobi coordinates for an equal mass A body system, with Cartesian coordinates $\mathbf{r}_1 \dots \mathbf{r}_A$

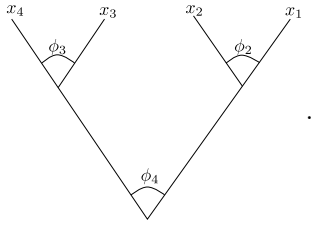
$$\mathbf{x}_{N-j+1} = \sqrt{\frac{2j}{j+1}}\,(\mathbf{r}_{j+1} - \mathbf{X}_j)\,, \qquad j = 1, \dots, N\,. \tag{1}$$

with $\mathbf{X}_j = \sum_{i=1}^{j} \mathbf{r}_j/j$. For a given set of Jacobi coordinates $\mathbf{x}_1, \dots, \mathbf{x}_N$, we can introduce the hyperspherical coordinates. A useful tool to represent hyperspherical coordinates is the hyperspherical tree. This is a rooted-binary tree whose leaves represent the modules of Jacobi coordinates. Once we introduce the hyperradius,

$$\rho = \left(\sum_{i=1}^{N} x_i^2\right)^{1/2} = \left(2\sum_{i=1}^{A}(\mathbf{r}_i - \mathbf{X})^2\right)^{1/2} = \left(\frac{2}{A}\sum_{j>i}^{A}(\mathbf{r}_j - \mathbf{r}_i)^2\right)^{1/2}, \tag{2}$$

the modulus of the Jacobi coordinates live in a $(N-1)$-sphere of radius ρ and we can introduce $N-1$ hyperangles to express the Jacobi coordinates as a function of the hyperradius. The choice is not unique, and different choices are represented by different hyperspherical trees [19,20]. The relation between a tree and the corresponding Jacobi coordinates is the following; for each tree's node, labelled by a, we have an hyperangle ϕ_a. The rule to reconstruct the value of a Jacobi coordinate modululs reads: start from the root node, and look for the path leading to the leaf corresponding to the Jacobi coordinate; for each branch turning toward the left (right) we multiply the hyperradius ρ for cosine (sine) of the hyperangle attached to the branching point. As an example, in Eq. (3) we have a tree choice for $A = 5$ with the corresponding relations between Jacobi and hyperspherical coordinates

$$\begin{aligned} x_1 &= \rho \sin\phi_4 \sin\phi_2 \\ x_2 &= \rho \sin\phi_4 \cos\phi_2 \\ x_3 &= \rho \cos\phi_4 \sin\phi_3 \\ x_4 &= \rho \cos\phi_4 \cos\phi_3\,, \end{aligned} \tag{3}$$



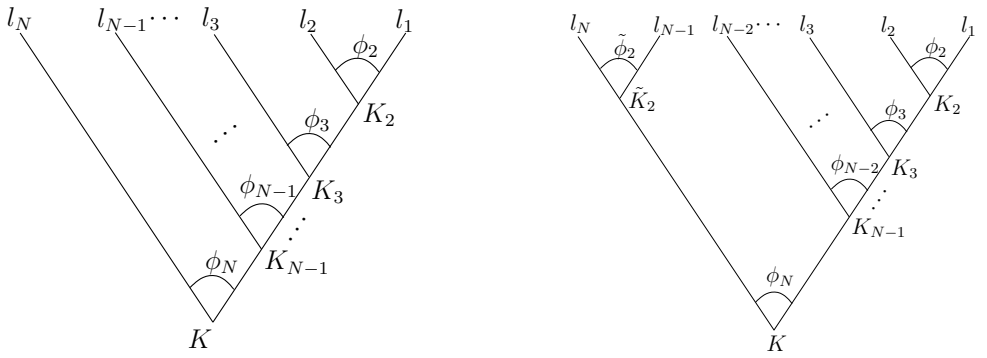


Fig. 1 In the left panel we have drawn the standard hyperspherical tree; this is the one used in the standard definition of the basis, and the one used to calculate the two-body potential between particles at $\mathbf{r}_1$ and $\mathbf{r}_2$. In the right panel we have drawn the non-standard tree, used to calculate the three-body force between particles at $\mathbf{r}_1$, $\mathbf{r}_2$, and $\mathbf{r}_3$.

Different trees have different topologies; given a node a, the left (right) branch connects the node to a sub-binary tree made up of $N_a^{l(r)}$ nodes and $L_a^{l(r)}$ leaves. We can use this information to construct useful topological numbers as

$$C_a = N_a^l + \frac{1}{2}L_a^l + \frac{1}{2}\,, \tag{4}$$

and

$$S_a = N_a^r + \frac{1}{2}L_a^r + \frac{1}{2}\,. \tag{5}$$

The set of the hyperangles together with the direction of the Jacobi coordinates $\hat{\mathbf{x}}_i = (\varphi_i, \theta_i)$ form the hyperangular coordinates

$$\Omega_N = (\hat{\mathbf{x}}_1, \ldots, \hat{\mathbf{x}}_N, \phi_2, \ldots, \phi_N)\,. \tag{6}$$

in terms of which the HH functions $\mathcal{Y}_{[K]}(\Omega_N)$ are defined. The subscript $[K]$ stands for the set of $(3N-1)$-quantum numbers $l_1, \ldots, l_N, m_1, \ldots, m_N, K_2, \ldots, K_N$, with $K_N = K$ the grand-angular momentum. They can be expressed in terms of the usual harmonic functions $Y_{lm}(\hat{\mathbf{x}})$ and of the Jacobi polynomials $P_n^{a,b}(z)$

$$\mathcal{Y}^{LM}_{[K]}(\Omega_N) = \left[\prod_{j=1}^{N} Y_{l_j m_j}(\hat{\mathbf{x}}_j)\right]_{LM} \left[\prod_{a\in\text{nodes}} \mathcal{P}_{K_a}^{\alpha_{K_a^l},\alpha_{K_a^r}}(\phi_a)\right], \tag{7}$$

with

$$\mathcal{P}_{K_a}^{\alpha_{K_a^l},\alpha_{K_a^r}}(\phi_a) = \mathcal{N}_{n_a}^{\alpha_{K_a^r},\alpha_{K_a^l}} (\cos\phi_a)^{K_a^l} (\sin\phi_a)^{K_a^r} P_{n_a}^{\alpha_{K_a^r},\alpha_{K_a^l}}(\cos 2\phi_a)\,, \tag{8}$$

where we have defined

$$\alpha_{K_a^{l(r)}} = K_a^{l(r)} + N_a^{l(r)} + \frac{1}{2}L_a^{l(r)}\,. \tag{9}$$

The normalization factor reads

$$\mathcal{N}_n^{\alpha\beta} = \sqrt{\frac{2(2n+\alpha+\beta+1)n!\,\Gamma(n+\alpha+\beta+1)}{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}}\,. \tag{10}$$

With the above definitions, the HH functions have well defined total orbital angular momentum L and z-projection M. The standard choice of hyperspherical coordinates, and of the corresponding HH, is represented in the left panel of Fig. 1; this is the one we use as our basis set.

2.2 Rotation matrices between HH basis elements of different Jacobi coordinates

Here we are interested in a particular set of coefficients relating the reference HH basis to a basis in which the ordering of two adjacent particles have been transposed. In the transposition between particles $j, j+1$, only the Jacobi vectors $\mathbf{x}_i$ and $\mathbf{x}_{i+1}$, with $i = N-j+1$, are different. We label them $\mathbf{x}'_i$ and $\mathbf{x}'_{i+1}$, and explicitly they are

$$\begin{aligned} \mathbf{x}'_i &= -\frac{1}{j}\,\mathbf{x}_i + \frac{\sqrt{(j+1)^2-2(j+1)}}{j}\,\mathbf{x}_{i+1} \\ \mathbf{x}'_{i+1} &= \frac{\sqrt{(j+1)^2-2(j+1)}}{j}\,\mathbf{x}_i + \frac{1}{j}\,\mathbf{x}_{i+1}\,, \end{aligned} \tag{11}$$

with $i = 1, \ldots, N-1$. The corresponding moduli verify $x'^2_i + x'^2_{i+1} = x^2_i + x^2_{i+1}$. Let us call $\mathcal{Y}^{LM}_{[K]}(\Omega^i_N)$ the HH basis element constructed in terms of a set of Jacobi coordinates in which the i-th and $i+1$-th Jacobi vectors are given from Eq.(11) with all the other vectors equal to the original ones (transposed basis). The coefficients

$$\mathcal{A}^{i,LM}_{[K][K']} = \int d\Omega_N [\mathcal{Y}^{LM}_{[K]}(\Omega_N)]^* \mathcal{Y}^{LM}_{[K']}(\Omega^i_N)\,, \tag{12}$$

are the matrix elements of a matrix $\mathcal{A}^{LM}_i$ that allows to express the transposed HH basis elements in terms of the reference basis. The total angular momentum as well as the grand angular quantum number K are conserved in the above integral ($K = K'$). The coefficients $\mathcal{A}^{i,LM}_{[K][K']}$ form a very sparse matrix and they can be calculated analytically using angular and $\mathcal{T}$-coupling coefficients (Kil'dyushov coefficients) and the Raynal-Revai matrix elements [11,21,18] .

We are now interested in obtaining the rotation coefficients between the reference HH basis and a basis in which the last Jacobi vector is defined as $\mathbf{x}'_N = \mathbf{r}_j - \mathbf{r}_i$, without loosing generality we consider $j > i$. A generic rotation coefficient of this kind can be constructed as successive products of the $\mathcal{A}^{k,LM}_{[K][K']}$ coefficients. Defining $\mathcal{Y}^{LM}_{[K]}(\Omega^{ij}_N)$ the HH basis element constructed in terms of a set of Jacobi coordinates in which the N-th Jacobi vector is defined $\mathbf{x}'_N = \mathbf{r}_j - \mathbf{r}_i$, the rotation coefficient relating this basis to the reference basis can be given in the following form

$$\mathcal{B}^{ij,LM}_{[K][K']} = \int d\Omega [\mathcal{Y}^{LM}_{[K]}(\Omega_N)]^* \mathcal{Y}^{LM}_{[K]}(\Omega^{ij}_N) = \left[\mathcal{A}^{LM}_{i_1} \cdots \mathcal{A}^{LM}_{i_n}\right]_{[K][K']}\,. \tag{13}$$

The particular values of the indices $i_1, \ldots, i_n$, labelling the matrices $\mathcal{A}^{LM}_{i_1}, \ldots, \mathcal{A}^{LM}_{i_n}$, depend on the pair (i, j). The number of factors cannot be greater than $2(j-2)$ and it increases, at maximum, by two units from j to $j+1$. The matrix

$$\mathcal{B}^{LM}_{ij} = \mathcal{A}^{LM}_{i_1} \cdots \mathcal{A}^{LM}_{i_n}\,, \tag{14}$$

is written as a product of the sparse matrices $\mathcal{A}^{LM}_i$'s, a property which is particularly well suited for a numerical implementation of the potential energy matrix.

2.3 The two-body and three-body potential energy matrices

We consider the potential energy of an A-body system constructed in terms of two-body interactions

$$V = \sum_{i<j} V(i,j) \quad . \tag{15}$$

In the case of a central two-body interaction, its matrix elements in terms of the HH basis are

$$V_{[K][K']}(\rho) = \sum_{i<j} \langle \mathcal{Y}^{LM}_{[K]}(\Omega_N) | V(i,j) | \mathcal{Y}^{LM}_{[K']}(\Omega_N) \rangle\,. \tag{16}$$

In each element $\langle \mathcal{Y}^{LM}_{[K]}|V(i,j)|\mathcal{Y}^{LM}_{[K']}\rangle$ the integral is understood on all the hyperangular variables and depends parametrically on ρ. Explicitly, for the pair $(1,2)$, the matrix elements of the matrix $V_{12}(\rho)$ are

$$\begin{aligned} &V^{(1,2)}_{[K][K']}(\rho) = \langle \mathcal{Y}^{LM}_{[K]}(\Omega_N)|V(1,2)|\mathcal{Y}^{LM}_{[K']}(\Omega_N)\rangle = \\ &\delta_{l_1,l'_1}\cdots\delta_{l_N,l'_N}\delta_{L_2,L'_2}\cdots\delta_{L_N,L'_N}\delta_{K_2,K'_2}\cdots\delta_{K_N,K'_N} \\ &\times \int d\phi_N (\cos\phi_N \sin\phi_N)^2 \ {}^{(N)}\mathcal{P}^{l_N,K_{N-1}}_{K_N}(\phi_N) V(\rho\cos\phi_N) \ {}^{(N)}\mathcal{P}^{l_N,K_{N-1}}_{K'_N}(\phi_N)\,. \end{aligned} \tag{17}$$

Using the rotation coefficients, a general term of the potential $V(i,j)$ results

$$V^{(i,j)}_{[K][K']}(\rho) = \sum_{[K''][K''']} \mathcal{B}^{ij,LM}_{[K''][K]} \mathcal{B}^{ij,LM}_{[K'''][K']} \langle \mathcal{Y}^{LM}_{[K'']}(\Omega^{ij}_N)|V(i,j)|\mathcal{Y}^{LM}_{[K''']}(\Omega^{ij}_N)\rangle\,. \tag{18}$$

or, in matrix notation,

$$V_{ij}(\rho) = [\mathcal{B}^{LM}_{ij}]^t \, V_{12}(\rho) \, \mathcal{B}^{LM}_{ij}\,. \tag{19}$$

The complete potential matrix energy results

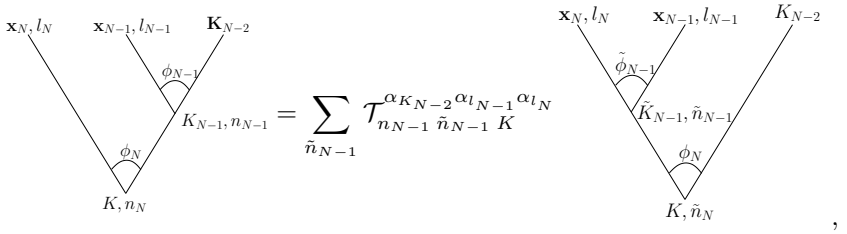
$$\sum_{i<j} V_{ij}(\rho) = \sum_{i<j} [\mathcal{B}^{LM}_{ij}]^t \, V_{12}(\rho) \, \mathcal{B}^{LM}_{ij}\,. \tag{20}$$

Each term of the sum in Eq.(20) results in a product of sparse matrices, a property which allows an efficient implementation of matrix-vector product, key ingredient in the solution of the Schrödinger equation using iterative methods.

The three-body force used in the present work depends on the hyperradius ρ_{ijk} of a triplet of particles $\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k$. For an A-body systems, there are $\binom{A}{3}$ three-body terms

$$V^{(3)} = \sum_{i<j<k} W(\rho_{ijk})\,, \tag{21}$$

and one of them is the force between the triplet $\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3$ for which we have $\rho^2_{123} = x^2_N + x^2_{N-1}$. This term can be easily calculated on a hyperspherical-basis set relative to an non-standard hyperspherical tree with the branches attached to leaves x_N and x_{N-1} going to the same node, as shown in the right panel of Fig. 1. The transition between this tree and the standard tree is simply given by the $\mathcal{T}$-coefficients



, (22)

or

$$\mathcal{Y}^{LM}_{[K]}(\Omega_N) = \sum_{\tilde{n}_{N-1}} \mathcal{T}^{\alpha_{K_{N-2}}\alpha_{l_{N-1}}\alpha_{l_N}}_{n_{N-1}\,\tilde{n}_{N-1}\,K} \mathcal{Y}^{LM}_{[\tilde{K}]}(\tilde{\Omega}_N)\,, \tag{23}$$

where all the variable with the tilde refer to the non-standard tree. In fact, with this choice we simply have

$$\rho_{123} = \rho\cos\phi_N\,, \tag{24}$$

and the fixed-rho matrix elements of the matrix $W_{123}(\rho)$ are

$$\begin{aligned} &\langle \mathcal{Y}^{LM}_{[\tilde{K}']}(\tilde{\Omega}_N)|W(\rho_{123})|\mathcal{Y}^{LM}_{[\tilde{K}]}(\tilde{\Omega}_N)\rangle = \\ &\delta_{l'_1,l_1}\cdots\delta_{l'_N,l_N}\delta_{L'_2,L_2}\cdots\delta_{L',L}\delta_{M',M}\delta_{\tilde{K}'_2,\tilde{K}_2}\cdots\delta_{\tilde{K}'_{N-1},\tilde{K}_{N-1}}\times \\ &\int (\cos\phi_N)^{C_K} (\sin\phi_N)^{S_K} d\phi_N \ \mathcal{P}_{K'}^{\alpha_{\tilde{K}_{N-1}},\alpha_{K_{N-2}}}(\phi_N) \mathcal{P}_{K}^{\alpha_{\tilde{K}_{N-1}},\alpha_{K_{N-2}}}(\phi_N) W(\rho\cos\phi_N)\,, \end{aligned} \tag{25}$$

where C_K and S_K are the topological quantum numbers relative to the grand-angular-K root node. In practice the matrix is extremely sparse, and it is diagonal on all quantum numbers but the grand-angular momentum.

The three-body force matrix in the standard basis is obtained by means of the $\mathcal{T}$-coefficients

$$\begin{aligned}&\langle \mathcal{Y}^{LM}_{[K']}(\Omega_N)|W(\rho_{123})|\mathcal{Y}^{LM}_{[K]}(\Omega_N)\rangle = \\ &\sum_{\tilde{n}_{N-1}} \mathcal{T}^{\alpha_{K_{N-2}}\alpha_{l_{N-1}}\alpha_{l_N}}_{n'_{N-1}\,\tilde{n}_{N-1}\,K'} \mathcal{T}^{\alpha_{K_{N-2}}\alpha_{l_{N-1}}\alpha_{l_N}}_{n_{N-1}\,\tilde{n}_{N-1}\,K} \langle \mathcal{Y}^{LM}_{[\tilde{K}']}(\tilde{\Omega}_N)|W(\rho_{123})|\mathcal{Y}^{LM}_{[\tilde{K}]}(\tilde{\Omega}_N)\rangle\,,\end{aligned} \tag{26}$$

which for all practical purposes reduces to a product of sparse matrices.

In order to calculate the other terms of the three-body force, we use the matrices $\mathcal{A}^{LM}_p$, defined in Eq. (12), that transpose particles; with a suitable product of these sparse matrices

$$\mathcal{D}^{LM}_{ijk} = \mathcal{A}^{LM}_{p_1} \cdots \mathcal{A}^{LM}_{p_m}\,, \tag{27}$$

we can permute the particles in such a way that $\mathbf{x}_N = \mathbf{r}_i - \mathbf{r}_j$, and $\mathbf{x}_{N-1} = 2/\sqrt{3}(\mathbf{r}_k - (\mathbf{r}_i + \mathbf{r}_j)/2)$, and $\rho^2_{ijk} = x^2_{N-1} + x^2_N$, and the total three-body force reads

$$V^{(3)} = \sum_{i<j<k} [\mathcal{D}^{LM}_{ijk}]^t\, W_{123}(\rho)\, \mathcal{D}^{LM}_{ijk}\,. \tag{28}$$

3 Applications of the HH expansion up to six particles

In this section we present results for $A = 3 - 6$ systems obtained by a direct diagonalization of the Hamiltonian of the system. The corresponding Hamiltonian matrix is obtained using the following orthonormal basis

$$\langle \rho\,\Omega\,|\,m\,[K]\rangle = \left(\beta^{(\alpha+1)/2}\sqrt{\frac{m!}{(\alpha+m)!}}\,L^{(\alpha)}_m(\beta\rho)\,\mathrm{e}^{-\beta\rho/2}\right)\mathcal{Y}^{LM}_{[K]}(\Omega_N)\,, \tag{29}$$

where $L^{(\alpha)}_m(\beta\rho)$ is a Laguerre polynomial with $\alpha = 3N-1$ and β a variational non-linear parameter. The matrix elements of the Hamiltonian are obtained after integrations in the ρ, Ω spaces. They depend on the indices m, m' and $[K], [K']$ as follows

$$\begin{aligned}\langle m'\,[K']|H|\,m\,[K]\rangle = &-\frac{\hbar^2\beta^2}{m}(T^{(1)}_{m'm} - K(K+3N-2)T^{(2)}_{m'm})\delta_{[K'][K]} \\ &+\sum_{i<j}\left[\sum_{[K''][K''']} \mathcal{B}^{ij,LM}_{[K][K'']}\mathcal{B}^{ij,LM}_{[K'''][K']}V^{m,m'}_{[K''][K''']}\right] \\ &+\sum_{i<j<k}\left[\sum_{[K''][K''']} \mathcal{D}^{ijk,LM}_{[K][K'']}\mathcal{D}^{ijk,LM}_{[K'''][K']}W^{m,m'}_{[K''][K''']}\right]\end{aligned} \tag{30}$$

.

The matrices $T^{(1)}$ and $T^{(2)}$ have an analytical form and are given in Ref. [11]. The matrix elements $V^{m,m'}_{[K][K']}$ are obtained after integrating the matrix $V_{12}(\rho)$ in ρ-space whereas the matrix elements $W^{m,m'}_{[K][K']}$ are obtained after integration of the matrix $W_{123}(\rho)$ (we will call the corresponding matrices V_{12} and W_{123}, respectively). Introducing the diagonal matrix D such that $\langle [K']\,|\,D\,|[K]\rangle = \delta_{[K],[K']}K(K+3N-2)$, and the identity matrix I in K-space, we can rewrite the Hamiltonian schematically as

$$H = -\frac{\hbar^2\beta^2}{m}({}^{(1)}T \otimes I + {}^{(2)}T \otimes D) + \sum_{ij}[\mathcal{B}^{LM}_{ij}]^t\, V_{12}\, \mathcal{B}^{LM}_{ij} + \sum_{ijk}[\mathcal{D}^{LM}_{ijk}]^t\, W_{123}\, \mathcal{D}^{LM}_{kij}\,, \tag{31}$$

in which the tensor product character of the kinetic energy is explicitly given.

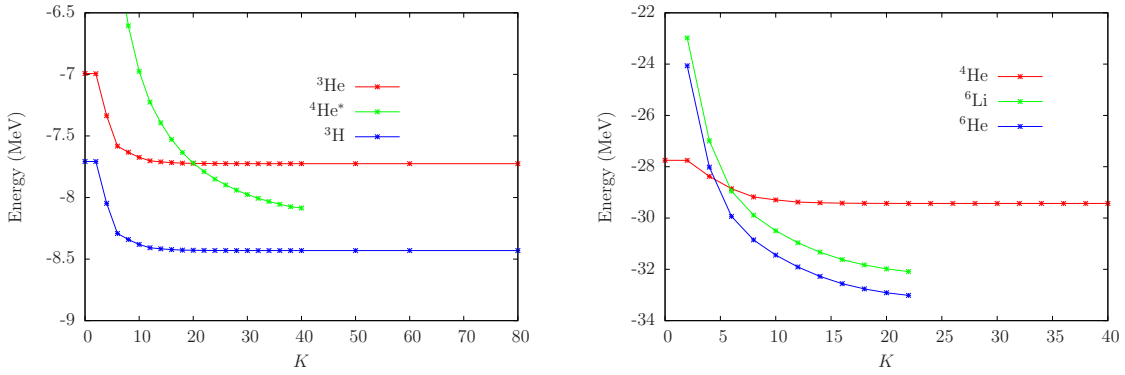


Fig. 2 In the left panel we have the convergence of the ^{3}H and ^{3}He binding energies as a function of K. The excited state of the alpha particle ^{4}He* is also shown. In the right panel we have the convergence of the ^{4}He, ^{6}He and ^{6}Li binding energies as a function of K.

3.1 nuclear system

As a first example we consider e nuclear system interaction through a simple two-body potential, the Volkov potential

$$V(r) = V_R \, \mathrm{e}^{-r^2/R_1^2} + V_A \, \mathrm{e}^{-r^2/R_2^2} \,, \tag{32}$$

with $V_R = 144.86$ MeV, $R_1 = 0.82$ fm, $V_A = -83.34$ MeV, and $R_2 = 1.6$ fm. The nucleons are considered to have the same mass chosen to be equal to the reference mass m and corresponding to $\hbar^2/m = 41.47$ MeV fm^2. With this parametrization of the potential, the two-nucleon system has a binding energy $E_{2N} = 0.54592$ MeV and a scattering length $a_{2N} = 10.082$ fm. This potential has been used several times in the literature making its use very useful to compare different methods [5, 8,9,10]. The use of central potentials in general produces too much binding, in particular the $A = 5$ system results bounded. Conversely, the use of the s-wave version of the potential produces a spectrum much closer to the experimental situation. This is a direct consequence of the weakness of the nuclear interaction in p-waves. Accordingly, we analyze this version of the potential, the s-wave projected potential. The results are obtained after a direct diagonalization of the Hamiltonian matrix of Eq.(30) including $m_{max} + 1$ Laguerre polynomials with a fix value of β, and all HH states corresponding to maximum value of the grand angular momentum K_{max}. The scale parameter β can be used as a non-linear parameter to study the convergence in the index $m = 0, 1, \ldots, m_{max}$, with m_{max} the maximum value considered. We found that 20 Laguerre polynomials (with proper values of β) were sufficient for an accuracy of 0.1% in the calculated eigenvalues.

The results of the present analysis are given in Fig. 2 where the convergence of the $A = 3 - 6$ binding energies are given as a function of K. In the left panel of Fig. 2 the convergence for the excited state ^{4}He* of the α particle is also shown. For $A = 3, 4$ a very extended HH expansion has been used with the maximum value of $K = 80$ and $K = 40$ respectively. For $A = 3$, the obtained results are 8.431 MeV and 7.725 MeV for ^{3}H and ^{3}He respectively. For $A = 4$, the ground state binding energy converges at the level of $1 - 2$ keV for $K_{max} = 40$. The convergence of the excited state ^{4}He* has been estimated at the level of 50 keV. Though the convergence was not completely achieved, the description is close to the experimental observation of a 0^+ resonance between the two thresholds and centered 395 keV above the p-^{3}H threshold. Besides its simplicity, the s-wave potential describes the $A = 3, 4$ system in reasonable agreement with the experiment.

For the $A = 6$ system a maximum value of $K = 22$ has been used which greatly improve previous attemps in using the HH basis in $A = 6$ systems [4,6]. The obtained results are 33.016 MeV and 32.087 MeV for ^{6}He and ^{6}Li respectively. It should be noticed that these states belong to the mixed symmetries $[\mathbf{4\,2}]$ (without the Coulomb interaction). When the Coulomb interaction between two nucleons is included the state belong to the symmetry $[\mathbf{2}] \otimes [\mathbf{2^2}]$ and when it is included between three nucleons the state belongs to the symmetry $[\mathbf{2\,1}] \otimes [\mathbf{2\,1}]$. These states are embedded in a very dense

spectrum. In order to follow these state in the projected Lanczos method a projection-purification procedure is performed.

3.2 atomic system

As an example of an atomic systems we describe a system of ^{4}He atoms up to six atoms. The ^{4}He-^{4}He interaction presents a strong repulsion at short distances, below 5 a.u. This characteristic makes it difficult a detailed description of the system with more than four atoms. Accordingly, we study small clusters of helium interacting through a soft-core two- and three-body potentials. Following Refs. [22, 17,18] we use the gaussian two-body potential

$$V(r) = V_0 \ \mathrm{e}^{-r^2/R^2} \ , \tag{33}$$

with $V_0 = -1.227$ K and $R = 10.03$ a.u.. In the following we use $\hbar^2/m = 43.281307$ (a.u.)^{2}K. This parametrization of the two-body potential approximately reproduces the dimer binding energy E_2, the atom-atom scattering length a_0 and the effective range r_0 given by the LM2M2 potential. Specifically, the results for the gaussian potential are $E_2 = -1.296$ mK, $a_0 = 189.95$ a.u. and $r_0 = 13.85$ a.u., to be compared to the corresponding LM2M2 values $E_2 = -1.302$ mK, $a_0 = 189.05$ a.u. and $r_0 = 13.84$ a.u.. As shown in Ref. [17], the use of the gaussian potential in the three-atom system produces a ground state binding energy $E_3^{(0)} = 150.4$ mK, which is appreciable bigger than the LM2M2 helium trimer ground state binding energy of 126.4 mK. In order to have a closer description to the $A = 3$ system obtained with the LM2M2 potential, we introduce the following three-body interaction

$$W(\rho_{ijk}) = W_0 \ \mathrm{e}^{-2\rho_{ijk}^2/\rho_0^2} \ , \tag{34}$$

where $\rho_{ijk}^2 = \frac{2}{3}(r_{ij}^2 + r_{jk}^2 + r_{ki}^2)$ is the three-body hyperradius in terms of the distances of the three interacting particles. Moreover, the strength W_0 is fixed to reproduce the LM2M2 helium trimer binding energy of 126.4 mK. In Ref. [18] a detailed analysis of this force has been performed by varying the range ρ_0 between 4 and 16 a.u.. Here we present results for small clusters, up to $A = 6$, formed by atoms of ^{4}He using the soft two-body force plus the hyperradial three-body force with parameters $W_0, \rho_0 \equiv 0.422\mathrm{K}, 14.0$ a.u..

The results are collected in Figs. 3,4 where we show the convergence in terms of K of the ground state and first excited state of the bosonic helium clusters. Starting from $A = 3$ the bosonic spectrum is formed by two states, one deep and one shallow close to the threshold formed by the $A - 1$ system with one atom far away. The calculations have been performed up to $K = 40$ in $A = 4$, $K = 24$ in $A = 5$ and $K = 22$ in $A = 6$. From the figure we can observe that the ground state binding energy, $E_A^{(0)}$, has a very fast convergence in terms of K. The convergence of the $E_A^{(1)}$ is much slower than for the ground state, however with the extended based used it has been determined with an accuracy well below 1%. The results confirm previous analyses in the four body sector that the lower Efimov state in the $A = 3$ system produces two bound states, one deep and one shallow. Here, we have extended this observation up to the $A = 6$ system. Specifically we have obtained the following ground state energies: $E_4^{(0)} = 568.8$ K, $E_5^{(0)} = 1326.6$ K,and $E_6^{(0)} = 2338.9$ K, and first excited state energies: $E_4^{(1)} = 129.0$ K, $E_5^{(1)} = 574.9$ K,and $E_6^{(0)} = 1351.6$ K. It is interesting to compare the results obtained using the soft-core representation of the LM2M2 potential with the results of Refs. [13,14] obtained using the original LM2M2 interaction. For the ground state the agreement is around 2% for $A = 4, 5$ and around 1% for $A = 6$. The agreement is worst for the excited state, however the results from Ref. [14] are obtained using approximate solutions of the adiabatic hyperspherical equations. The recent, and very accurate, results of Ref. [15] for $A = 4$ ($E_4^{(0)} = 558.98$ K and $E_4^{(1)} = 127.33$ K) shows a good agreement in particular for the first excited state.

Finally it is possible to analyze the ratios $E_A^{(1)}/E_{A-1}^{(0)}$. In the case of Efimov physics these ratios present and universal character. The He-He potential it is not located exactly at the unitary limit (infinite value of a_0) but it is close to it. Using the soft potential models these ratios are: $E_4^{(1)}/E_3^{(0)} = 1.020$, $E_5^{(1)}/E_4^{(0)} = 1.011$ and $E_6^{(1)}/E_5^{(0)} = 1.018$. The ratios between the trimer ground state and the ground states of the $A = 4, 5, 6$ systems are $E_4^{(0)}/E_3^{(0)} = 4.5$, $E_5^{(0)}/E_3^{(0)} = 10.5$ and $E_5^{(0)}/E_3^{(0)} = 18.5$, respectively. These ratios are in good agreement with those given in Refs. [23,24,25].

The overall agreement of the $A = 4, 5, 6$ systems between LM2M2 and the soft potential model gives a further indication that these systems are a nice realization of which it is called Efimov physics.

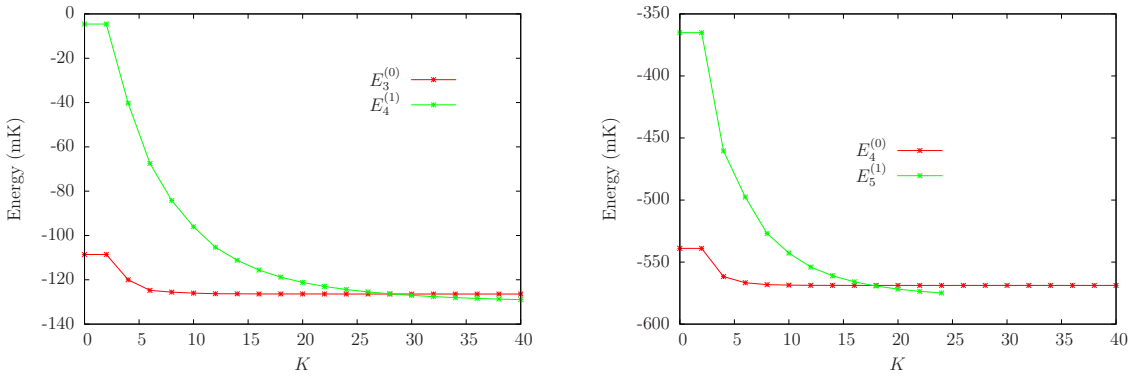


Fig. 3 The trimer bound state and tetramer first excited state (left panel) and tetramer bound state and pentamer first excited state (right panel) as a functions of K.

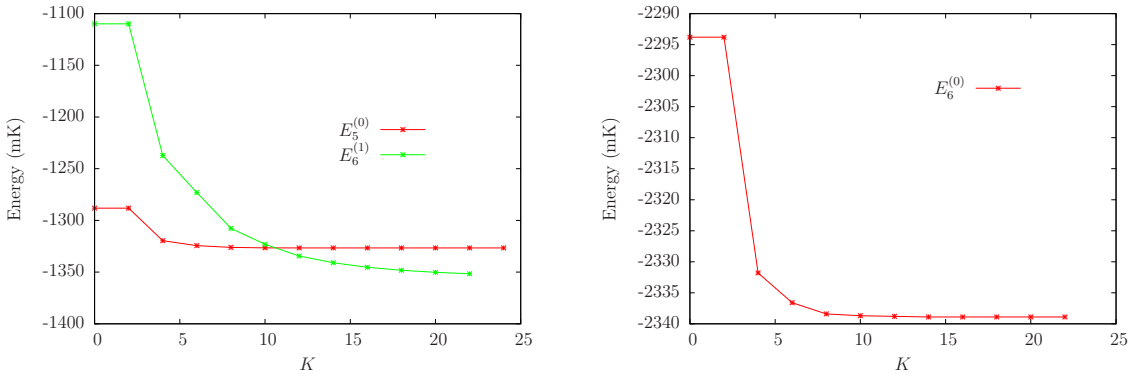


Fig. 4 The pentamer bound state and hexamer first excited state (left pannel) and hexamer bound state (right pannel) as a functions of K.

4 Conclusions

In this work we have shown results using the HH expansion in the description of a A-body system with $A = 3-6$. The basis has not been symmetrized or antisymmetrized as required by a system of identical particles. However, the eigenvectors of the Hamiltonian have well defined permutation symmetry. The benefit of the direct use of the HH basis is based on a particular simple form used to represent the potential energy. We have limited the analysis to consider a central potential. In a first example we have describe a system of nucleons interacting through the Volkov potential, used several times in the literature. Though the use of a central potential leads to an unrealistic description of the light nuclei structure, the study has served to analyze the characteristic of the method: the capability of the diagonalization procedure to construct the proper symmetry of the state and the particular structure, in terms of products of sparse matrices, of the Hamiltonian matrix. The success of this study makes feasible the extension of the method to treat interactions depending on spin and isospin degrees of freedom as the realistic NN potentials. A preliminary analysis in this direction has been done [26].

In a second example we have studied the possibility of calculating bound and excited states in a bosonic system consisting of helium atoms interacting through soft two- and three-body forces. The

potential model has been adjusted to approximate the description of small helium clusters interacting through one of the realistic helium-helium interactions, the LM2M2 potential. After the direct diagonalization of the A-body system we have observed that clusters with $A = 3, 4, 5, 6$ atoms present a deep bound state and a shallow bound state just below the energy of the $A-1$ system. Since the He-He potential predicts a large two-body scattering length we have studied the universal ratios $E_A^{(1)}/E_{(A-1)}^{(0)}$. These ratios have been studied in detail in the $A = 4$ case (see Refs. [27,24]). Estimates have been obtained also for bigger systems [25]. Our calculations, obtained for one particular value of the ratio r_0/a, are in agreement with those ones. An analysis of the universal ratios as $a \to \infty$ is at present under way.

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